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ABSTRACT

We discuss approximation techniques for estimating spatially varying coefficients and unknown boundary parameters in second order hyperbolic systems. Methods for state approximation (cubic splines, tau-Legendre) and approximation of function space parameters (interpolatory splines) are outlined and numerical findings for use of the resulting schemes in model "1-D seismic inversion" problems are summarized.

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1. Introduction. We discuss here some of our continuing efforts on the development of computational techniques for estimation or "identification" of parameters in second order hyperbolic systems (e.g., the acoustic wave equation). The parameters of interest include boundary parameters such as coefficients of elasticity and source terms in elastic boundary conditions as well as spatially varying moduli of elasticity in the partial differential equation itself. Among the features of our approach are the following: We do not require an impulse or delta function for the source term; indeed the source term need not even be parameterized a priori (although it is in the numerical examples presented below). Furthermore, the elastic moduli in the system equations can be estimated with or without a priori parameterization (i.e., assumption of a specific form or shape class). Our ideas are, in principle, applicable to vector systems in appropriately defined multidimensional domains.

We combine results from the theory of dissipative operators, linear semigroups, approximation theory (splines, spectral methods), and optimization techniques in our attempts to develop theoretically sound and numerically attractive procedures. While our long term goals include development of efficient methods for use in 2-D and 3-D problems such as those that arise in "surface seismic" and "bore hole" inversion (we have made progress in this direction), we illustrate some of our ideas here with a scalar "model problem" in 1-D. The system in this model problem is given by

$$(1) \quad \rho(x)u_{tt} = \frac{\partial}{\partial x}\left(E(x)\frac{\partial u}{\partial x}\right), \qquad 0 \le x \le 1, \quad t > 0$$

$$(2) \quad u_x(t,0) + k_1 u(t,0) = S(t,\tilde{q}),$$

$$(3) \quad u_t(t,1) + k_2 u_x(t,1) = 0,$$

$$(4) \quad u(0,x) = 0, \quad u_t(0,x) = 0.$$

Here ρ is the medium mass density and E is an elastic modulus in (1) while the boundary condition (2) is an elastic surface $(x=0)$ condition involving a restoring force parameter k_1 as well as a parameter $(\tilde{q})$ dependent source term S. This source term is assumed to be the result of a perturbing shock to the medium which occurs on the surface at some distance from the point of observation. The medium is initially at rest (initial conditions (4)) and it is assumed that no waves are reflected at a finite lower boundary $(x=1)$; this is given by the absorbing boundary condition (3)--(this condition can be obtained formally by factoring the equation (1) at $x=1$ and taking $k_2 = \sqrt{E(1)/\rho(1)}$). We make the physically motivated assumptions $k_1 < 0$, $k_2 > 0$ throughout.

Our model problem consists of using observations of the system (1) - (4) to estimate the parameters $q = (\rho, E, k_1, k_2, \tilde{q})$. More precisely we consider the mathematical problem of minimizing the fit-to-data criterion

$$(5) \qquad J(q) = \sum_{i,j} |u(t_i, x_j; q) - \hat{y}_{ij}|^2$$

over a given admissible parameter set Q. Here we assume we have observations $\hat{y}_{ij}$ for $u(t_i, x_j)$--(the "bore hole" problem)--or for $u(t_i, 0)$--(the "surface seismic" problem), where u is the solution to (1) - (4) corresponding to q.

It is convenient for our theoretical discussions to reformulate this problem in terms of an abstract evolution equation in a Hilbert space. To do this we first assume that the system (1) - (4) has been transformed to a system with homogeneous boundary conditions

$$\rho v_{tt} = \frac{\partial}{\partial x}\left(E \frac{\partial v}{\partial x}\right) + g(t,x,q)$$

$$(6) \qquad \begin{aligned} &v_x(t,0) + k_1 v(t,0) = 0 \\ &v_t(t,1) + k_2 v_x(t,1) = 0 \\ &v(0,x) = \phi(x,q), \quad v_t(0,x) = \psi(x,q) \, . \end{aligned}$$

This can be done in a straightforward fashion (see [11]).

As our state space we choose $Z = H^1(0,1) \times H^0(0,1)$ with parameter dependent inner product

$$\langle z,w\rangle_q = \int_0^1 E z_1' w_1' dx - E(0)k_1 z_1(0)w_1(0) + \int_0^1 \rho z_2 w_2 dx ,$$

for $z = (z_1,z_2)$, $w = (w_1,w_2)$ in Z. Under reasonable assumptions on ρ, E and k_1, this yields a Hilbert space $Z = Z(q)$ with topology equivalent to the usual $H^1 \times H^0$ topology. The transformed system (6) can then be written in abstract form as (we don't distinguish between a vector and its transpose)

$$(7) \qquad \begin{aligned} \dot{z}(t) &= A(q)z(t) + G(t,q) \\ z(0) &= \Phi(q) \end{aligned}$$

where $z = (v,v_t)$, $\Phi = (\phi,\psi)$, $G = (0,g)$, and the operator $A(q)$ defined on $\mathrm{dom}(A(q)) = \{z \in H^2 \times H^1 \mid z_1'(0) + k_1 z_1(0) = 0,\ z_2(1) + k_2 z_1'(1) = 0\}$ is given by

$$A(q) = \begin{pmatrix} 0 & 1 \\ \frac{1}{\rho}\frac{\partial}{\partial x}\left(E\frac{\partial}{\partial x}\right) & 0 \end{pmatrix} .$$

It can then be shown that under boundedness assumptions on Q, there exists a constant ω independent of q in Q such that $A(q) - \omega I$ is dissipative in Z (i.e., $\langle A(q)z,z\rangle \le \omega\langle z,z\rangle$). Furthermore $A(q)$ generates a strongly continuous semigroup $S(t;q)$, $t \geq 0$, that is the family of solution operators for (7).

This framework provides a convenient setting for discussion of semidiscrete approximation schemes (and their convergence properties) for solving the problem of minimizing (5) over Q. In the case under consideration here both the state space for (1) - (4) and the parameter set Q are infinite dimensional. We first turn to a description of <u>state approximation</u> ideas that we have employed.

Abstractly, one approximates (7)--at least in its state variable--by choosing a sequence of finite dimensional subspaces Z^N, $N = 1,2,\ldots$, of the state space Z. Letting P^N be the projection of Z onto Z^N and $A^N : Z^N \to Z^N$ be a family of approximating operators for A, one can define the sequence of approximating systems in Z^N by

$$\text{(8)} \qquad \begin{aligned} \dot{z}^N(t) &= A^N(q)z^N(t) + P^N G(t,q) \\ z^N(0) &= P^N \Phi \end{aligned}$$

and the corresponding fit-to-data criterion

$$\text{(9)} \qquad J^N(q) = \sum_{i,j} |z_1^N(t_i)(x_j) - \hat{y}_{ij}|^2 .$$

The problem of minimizing J^N over Q is then a finite dimensional state problem which can in some cases (e.g., when the functional parameters are assumed in parameteric form) be readily solved for approximate parameters $\bar{q}^N$, $N = 1,2,\ldots$. In this situation one then desires to argue that the sequence $\{\bar{q}^N\}$ (or some subsequence) converges to a parameter q^* in Q that provides a minimum for (5). However, in other cases where the parameter functions (such as ρ and E in (1)) are not assumed to possess a priori finite dimensional parameterizations, the problems involving (8), (9) still entail optimizations over an infinite dimensional set and thus a parameter approximation scheme must further be introduced before the approximating problems are easily solved. We defer discussion of this aspect of our methods until section 4 below. Instead we first discuss two state approximation schemes (cubic spline and tau-Legendre) that we have used with some success.

2. Cubic spline state approximations. These methods are founded on ideas given in [1],[3],[9] where cubic B-splines $\hat{B}_j^N$ (see [13] for general concepts and discussions) are used to generate basis elements for subspaces Z^N in which the elements satisfy the boundary conditions inherent in the problem. For the problems under consideration in this note, this results in parameter dependent basis elements $B_j^N = B_j^N(q)$. Thus the dependence of $Z^N = Z^N(q)$ on q is not only because of the parameter dependent inner product but also through the explicit

dependence of the basis elements B_j^N on the parameters. This aspect leads to nontrivial technical difficulties (from both a theoretical and a numerical viewpoint) in extending the ideas of [3]. One can however overcome these difficulties to obtain a theoretically sound and computationally feasible scheme (see [8], [11] for more detailed discussions).

To give a brief idea of the theoretical aspects of this method, we first observe that the above considerations lead to subspaces $Z^N = Z^N(q)$ in the context of the Galerkin approach of [3], [7]. One then desires to define Galerkin approximations $A^N = A^N(q^N) = P^N(q^N)A(q^N)P^N(q^N)$ associated with a given sequence of parameter estimates $\{q^N\}$. Here $P^N(q)$ is the orthogonal projection of $Z(q)$ onto $Z^N(q)$. To establish a state convergence theory for (8), it suffices to argue stability and consistency for the schemes (see [3], [7]). Stability follows readily from the uniform dissipativeness of the operators $A(q): \langle A^N(q)z,z\rangle = \langle P^N(q)A(q)P^N(q)z,z\rangle = \langle A(q)P^N(q)z,P^N(q)z\rangle \leq \omega\langle P^N(q)z,P^N(q)z\rangle \leq \omega\langle z,z\rangle$. Consistency is somewhat more delicate since one wishes to argue that for $q^N \to q^*$ in Q one has $A^N(q^N)z \to A(q^*)z$. More generally in the process of discussing consistency and state convergence one must deal with statements involving the convergence of elements z^N in $Z^N(q^N)$--which satisfy boundary conditions involving q^N--to elements z^* in $\mathrm{dom}(A(q^*))$. Hence one must construct some device to express convergence of the boundary condition parameters as well as that of the parameters defined directly in the operators $A^N(q^N)$. With care this can be done and one can employ the Trotter-Kato approximation theorem from linear semigroup theory [12] along with estimates from spline approximation theory [13] to establish consistency and state convergence (see [8], [11] for details).

These spline based schemes have proven quite satisfactory in numerical computations with test examples as we shall see in the numerical section below.

3. <u>Tau-Legendre state approximations</u>. The tau method (due to Lanczos) is a special case (see p. 11 of [10]) of the spectral methods discussed in [10] and involves use of eigenfunctions that are in general <u>not</u> related to the natural modes of the system being approximated. As outlined above, one again rewrites the system (6) as an abstract system in the state space $Z = Z(q)$ defined in section 1. The system (7) is written in the form

$$\text{(10)}\qquad \begin{aligned} \dot{z}(t) &= L(q)z(t) + G(t,q) \\ z(0) &= \Phi(q) \end{aligned}$$

(11) $\mathcal{B}(q)z(t) = 0$,

where $L(q)$ is the same as the operator $\mathcal{A}(q)$ in (7) except that we do not include the boundary conditions in defining the domain of $L(q)$; i.e., $\mathrm{dom}(L(q)) = H^2 \times H^1$. Instead the boundary operations are imbedded in an operator $\mathcal{B}$ and we impose the side conditions (11).

The approximating subspaces Z^N are then defined in terms of an orthonormal family that is complete in $H^0(0,1)$. Members in this family are not required to individually satisfy the boundary conditions; these are imposed on the approximations to the solution of (10), (11) by requiring that the approximations satisfy exactly the conditions (11). To be more specific, suppose we begin with $N+1$ elements $\{\phi_1,\ldots,\phi_{N+1}\}$ (e.g., Legendre functions) to generate the appropriate subspaces $Z^N(q)$ of $Z(q)$--(the $Z^N(q)$ have dimension $2N = (N+1) + (N-1)$ in this case--the analogous cubic spline approximating subspaces have dimension $2N+3$). Then we assume that the first components of solutions $z = (v,v_t)$ of (10)--i.e., of (6)--are approximated by $v^N(t,x) = \sum_{j=1}^{N+1} w_j(t)\phi_j(x)$ where the first $N-1$ coefficients w_j are determined by imposing the equation (10) and the remaining coefficients are determined by imposing the boundary conditions (11).

We observe that the tau method is not a Galerkin procedure. It also differs from the cubic spline method described above in that the approximating subspaces satisfy $Z^N \subset Z^{N+K}$, $K > 0$.

Our efforts have been devoted to the use of the tau-Legendre method in the model problem of section 1. In this case, we chose $\phi_j(x) = P_{j-1}(2x-1)$, $0 \le x \le 1$, $j = 1,2,\ldots,N+1$, where P_j is the Legendre polynomial of degree j. For a convergence analysis, one can employ the same Hilbert space framework described in discussing the cubic spline schemes. In this operator formulation one again establishes convergence via demonstrating stability and consistency. The arguments involve dissipative estimates, the Gronwall inequality, and approximation properties of Legendre polynomials.

One interesting (and potentially highly advantageous) aspect of the tau-Legendre methods involves their use in layered media problems (e.g., see Example 4 below) where the coefficients ρ, E in (1) possess discontinuities. In this case one can include (in addition to the boundary conditions) in the conditions (11) the continuity conditions $v^N(t,x_j^-) = v^N(t,x_j^+)$--on displacement--and $E(x_j^-)v_x^N(t,x_j^-) = E(x_j^+)v_x^N(t,x_j^+)$--on stress--at interfaces x_j in the medium. This

could lead to methods that are computationally superior to methods in which these interface continuity conditions are imposed directly on the basis elements for Z^N.

4. Parameter approximations. As we have noted above, the problem of minimizing J^N of (9) over Q subject to the state approximation equations (8) is still a difficult infinite dimensional optimization problem in cases where Q has nonparameterized function space components (e.g., in situations where we estimate ρ and/or E in (1) choosing from some infinite dimensional function classes). In such situations it is useful to introduce a family of finite dimensional parameter sets Q^M that approximate, in some sense, the original parameter set Q--i.e., "$Q^M \to Q$" as $M \to \infty$. We may then consider the problem of minimizing J^N of (9) over Q^M, which is finite dimensional in both the states and parameters and may be easily solved for judicious choices of Q^M, producing estimates $\bar{q}_M^N$.

We have, with some success, used such double approximation procedures to estimate functional coefficients in parabolic transport equations [4], [5], [6] and in higher order equations of elasticity [2]. In these efforts we employed approximating sets Q^M consisting of either linear or cubic interpolatory splines. Under reasonable assumptions on Q and on the approximation properties of Q^M (e.g., see [2], [4], [6] where theoretical results are also given for the systems mentioned above), one can prove a double limit convergence result: Given any sequence of estimates $\{\bar{q}_M^N\}$ as defined above, there exists a subsequential limit $q^* = \lim \bar{q}_{M_j}^{N_k}$ in Q that provides a minimum for J of (5) over Q.

In the next section we shall present a sample of some of our numerical results using such procedures.

5. Numerical examples. We present here a summary of some of our numerical findings for the methods described above when used with the model problem involving (1) - (5). The estimation schemes were tested on examples in the following manner. First, known "true" values (denoted by q^* in the tables below) of the parameters to be estimated were chosen and a numerical method independent of the one being tested was used to solve the forward problem for a solution $u = u(q^*)$. Values of this numerical solution were used for "observations" or data for the inverse algorithm. The minimization problems were solved iteratively (with "start-up" or initial guess q^0 listed in each example) employing an IMSL version (ZXSSQ) of the Levenberg-Marquardt algorithm. The ordinary differential equations for the approximate states were

solved using either DVERK or DGEAR in the IMSL packages. The test calculations were carried out on an IBM 370 at Brown University, a CDC 6600 at Southern Methodist University, and CDC Cyber 170 at NASA Langley Research Center. In the first two examples we compare the cubic spline state approximation scheme with the one based on tau-Legendre state approximations. In the third example we give a sample of our findings on a problem where the double approximation ideas of section 4 were used while in the last example we detail results for a multilayered media problem.

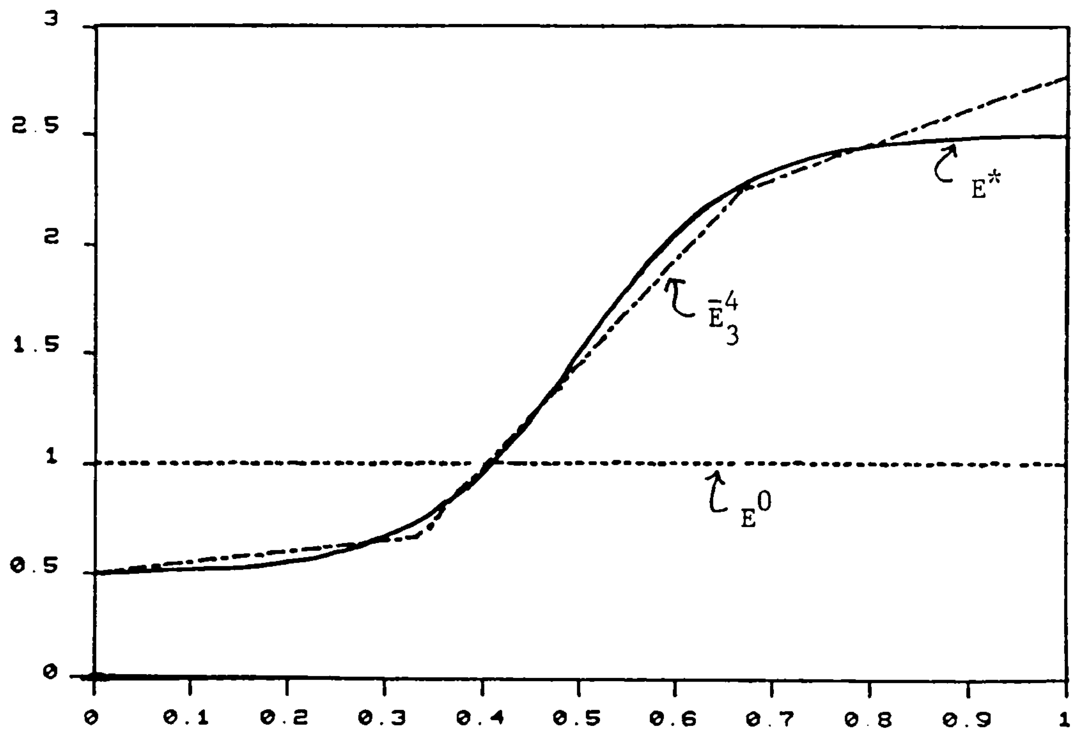
Example 1. In this example we considered (1) - (4) with $E/\rho = q_1$ constant, source $S(t,\tilde{q}) = q_2(1-e^{-5t})e^{q_3 t}$ and k_1, k_2 to be estimated. The "true" values q^*, start-up values q^0, along with findings for the cubic spline state approximations and the tau-Legendre state schemes are given below in tabular form. Observations included values $u(t_i,x_j;q^*)$ for t_i values .5, 1 and 1.5, x_j values 0, .5, and 1. The residual $(J^N(\bar{q}^N))$ for the converged parameter values along with CPU time in seconds is listed for each level (N) of state approximation.

	$\bar{q}_1^N$	$\bar{q}_2^N$	$\bar{q}_3^N$	$\bar{k}_1^N$	$\bar{k}_2^N$	$J^N(\bar{q}^N)$	CPU
CUBIC SPLINES							
N = 4	3.014	2.001	-1.084	-1.883	.992	$.6\text{x}10^{-5}$	124
N = 8	2.992	2.017	- .958	-2.082	.999	$.17\text{x}10^{-5}$	108
TAU-LEGENDRE							
N = 4	2.940	2.098	-1.026	-2.034	.994	$.7\text{x}10^{-3}$	31
N = 8	3.017	1.957	-1.001	-1.979	1.008	$.6\text{x}10^{-5}$	40
TRUE VALUES (q^*)	3.0	2.0	-1.0	-2.0	1.0		
START UP (q^0)	2.0	1.5	- .5	-1.0	2.0		

Example 2. We considered the transformed system (6) with $\rho = 1$, $g = 0$, parameterized modulus $E(x) = 1.5 + \frac{1}{\pi}$ Arctan $(q_1(x - q_2))$ and initial data $\phi(x) = e^x$, $\psi(x) = - 3e^x$. Observations at values $t_i = .16, .33, .5, .66, .83, 1$ and $x_j = 0, .5, 1$ were used. The following converged values were obtained.

	$\bar{q}_1^N$	$\bar{q}_2^N$	$\bar{k}_1^N$	$\bar{k}_2^N$	$J^N(\bar{q}^N)$	CPU
CUBIC SPLINES						
N = 4	2.964	.487	-.990	3.006	$.8\times10^{-4}$	60
N = 8	3.051	.501	-.999	2.996	$.28\times10^{-5}$	54
N = 16	3.012	.5002	-.9999	2.999	$.19\times10^{-6}$	146
TAU LEGENDRE						
N = 4	3.191	.516	-1.028	3.015	$.12\times10^{-2}$	14
N = 8	2.942	.496	-1.001	2.997	$.8\times10^{-4}$	57
N = 16	2.991	.4992	- .9998	2.999	$.15\times10^{-5}$	520
TRUE VALUES (q^*)	3.0	.5	-1.0	3.0		
START UP (q^0)	5.0	1.0	-2.0	2.0		

Example 3. We considered the system (6) with $\rho = 1$, $g = 0$, $\phi(x) = e^x$, $\psi(x) = -3e^x$ and parameters to be estimated $E^*(x) = 1.5 + \tanh(6(x-.5))$, $k_1^* = -1.0$, $k_2^* = 3.0$. We did not assume an a priori parameterization for E, but used linear interpolatory splines for the parameter approximation procedure as described in section 4. Cubic spline state approximations were used. Observations were taken at the same t_i, x_j as in Example 2. The initial guesses were $E^0(x) = 1.0$ (a constant function), $k_1^0 = -2.0$, $k_2^0 = 2.0$. Graphs for $\bar{E}_M^N$ are given in the figures below for N = 4 (2N + 3 = 11 cubic elements in the basis for Z^N) and N = 16 with parameter approximations corresponding to M = 3 (M + 1 = 4 linear elements to approximate E). For N = 4, the results obtained were $\bar{k}_1^4 = -1.054$, $\bar{k}_2^4 = 3.357$, $J^4(\bar{q}^4) = .25\times10^{-2}$, $|E^* - \bar{E}_3^4| = .81\times10^{-1}$, CPU = 38 sec., while for N = 16 the results were $\bar{k}_1^{16} = -1.100$, $\bar{k}_2^{16} = 3.070$, $J^{16}(\bar{q}^{16}) = .47\times10^{-4}$, $|E^* - \bar{E}_3^{16}| = .29\times10^{-1}$, CPU = 118 sec.


3
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0
0.1
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0.5
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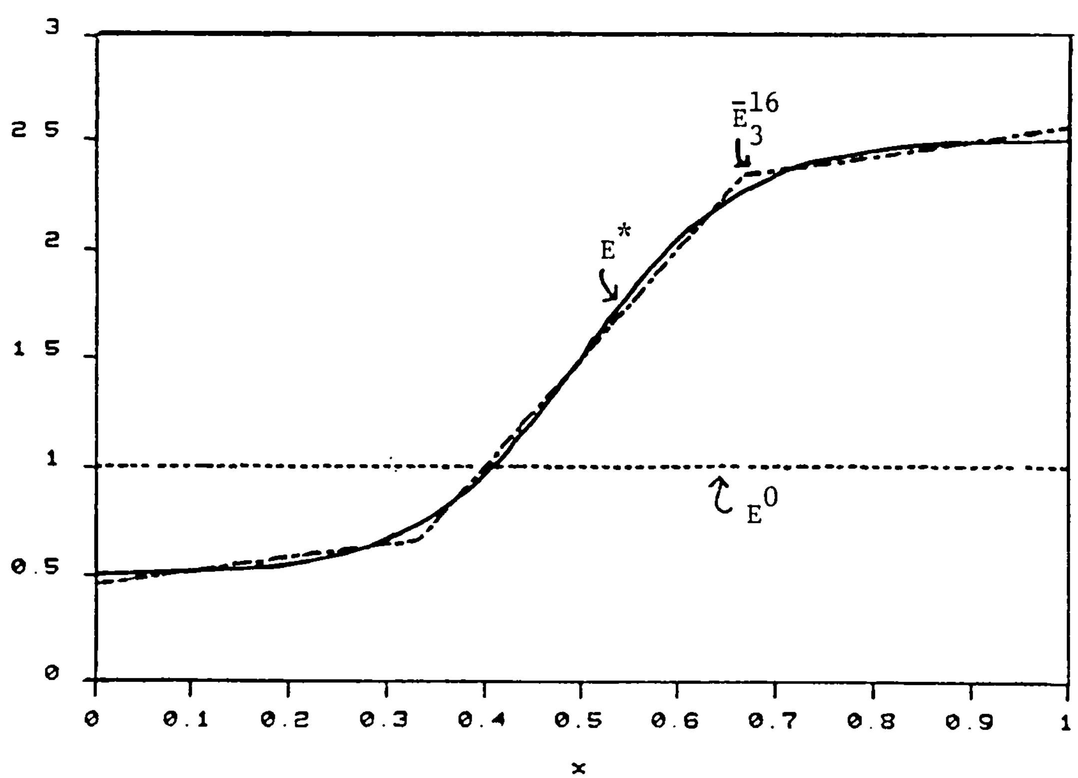
0.7
0.8
0.9
1
E^*
$\bar{E}_3^4$
E^0


3
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0.8
0.9
1
x
$\bar{E}_3^{16}$
E^*
E^0

Example 4. We considered system (1) - (4) for a multilayered medium (i.e., a discontinuous elastic modulus). We chose $\rho = 1$, E piecewise constant (E^* given below) and $S = 2(1 - e^{-5t})e^{-t}$ and used the tau-Legendre method for the state approximations as described in section 3 to estimate E, k_1, k_2. Observations consisted of surface observations ($x_j = 0$) at 40 evenly spaced times t_i in $[0,2]$ (i.e., $t_i = .05, .1, .15, \ldots$). For N = 4, we obtained the estimates listed below with $J^4(\bar{q}^4) = .3\text{x}10^{-3}$, CPU time = 172 sec.

INITIAL GUESS

$$E^0(x) = \begin{cases} 1.5 & 0 \le x \le .2 \\ 1.5 & .2 < x \le .8 \\ 1.5 & .8 < x \le 1.0 \end{cases} \qquad k_1^0 = -2.0, \quad k_2^0 = 2.0$$

TRUE VALUES

$$E^*(x) = \begin{cases} 2.0 & 0 \le x \le .3 \\ 3.0 & .3 < x \le .7 \\ 1.0 & .7 < x \le 1.0 \end{cases} \qquad k_1^* = -1.0, \quad k_2^* = 3.0$$

ESTIMATES (N = 4)

$$\bar{E}^4(x) = \begin{cases} 1.996 & 0 \le x \le .299 \\ 2.986 & .299 < x \le .7006 \\ .996 & .7006 < x \le 1.0 \end{cases} \qquad \bar{k}_1^4 = -.998, \quad \bar{k}_2^4 = 2.987$$

Concluding remarks. As we have outlined above, a convergence theory can be developed for both the state and parameter approximation schemes described in this note. We have tested the methods on a number of examples in addition to the ones presented here. The schemes perform well on both "bore hole" and "surface seismic" type model problems. In some cases (see Example 1) the tau-Legendre state approximations perform slightly better than the cubic spline approximations. In others (see Example 2), the cubic spline schemes appear to be more desirable.

While our test examples are clearly very simple, they do serve the purpose of illustrating the potential for use of the methods and ideas

in estimating variable (continuous and/or discontinuous) coefficients and unknown boundary parameters in second order hyperbolic systems.

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16. Abstract

We discuss approximation techniques for estimating spatially varying coefficients and unknown boundary parameters in second order hyperbolic systems. Methods for state approximation (cubic splines, tau-Legendre) and approximation of function space parameters (interpolatory splines) are outlined and numerical findings for use of the resulting schemes in model "1-D seismic inversion" problems are summarized.

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